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Towards Novel Alkaline Earth Metal Pyrazolates: Opportunities in Materials Chemistry

A Capstone Project Submitted in Partial Fulfillment of the Requirements of the Renée Crown University Honors Program at Syracuse University

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Honors Capstone Project in Chemistry

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Abstract:

Until recent years, the coordination chemistry of the alkaline earth metals remained relatively unexplored. Owing to the development of new synthetic methods and improved techniques for the exclusion of air and moisture, great progress has been made into our understanding of the alkaline earth metals and their compounds. These compounds are useful in a wide variety of applications, including as polymerization initiators, precursors for chemical vapor deposition (CVD) and in metal-organic frameworks (MOFs) for gas separation and storage. Current work in alkaline earth metal chemistry focuses on designing and tailoring ligand systems to expand their potential applications in materials chemistry.

The pyrazole ligand system, previously explored in alkaline earth chemistry, becomes a promising candidate, due to its facile synthesis and substitution and the variety of available binding modes with which coordinative saturation of the metal can be achieved. One novel approach includes introducing "pendant arms," extended substituents in the 3 and 5 positions, capable of stabilizing metal centers through potential Lewis base donation. These pendant arm pyrazoles are applicable in the synthesis of CVD precursors. Current precursors often contain neutral donors which can cause premature decomposition upon heating, therefore reducing or eliminating the need for donors by utilizing pendant arms is advantageous.

Also of interest is the synthesis of potential alkaline earth metal-organic frameworks for hydrogen storage. 2-D geometry can be introduced into the target MOFs by synthesizing bidentate dipyrazole ligands, allowing them to act as "linkers" between adjacent metal nodes. Furthermore, the pyrazole substituents can be modified in order to introduce intermolecular stabilizing forces and tune pore sizes. A novel ligand, 3,5,3',5'-tetraphenyl-1,4-xylylene-4,4'-dipyrazole, has been synthesized to explore the effect of these substituents on metal-organic frameworks.

This work presents novel approaches in the design and preparation of ligands for the aforementioned applications. The utility of alkaline earth metal compounds for these applications may be enhanced through the utilization of these new ligands. This work also presents novel applications of synthetic routes toward the preparation of alkaline earth organometallic compounds.